CLAIMS

What is claimed is:

1. An ErbB4 kinase domain in liganded crystalline form, comprising the amino acid sequence of SEQ ID NO: 1 and having the structural coordinates of Table 2.

2. A liganded ErbB4 kinase domain as claimed in claim 1, wherein the crystalline form has lattice constants of a = 63.95 Å, b = 63.95 Å, c = 163.95 Å, $\alpha = 90°$, $\beta = 90°$, and $\gamma = 90°$.

3. A liganded ErbB4 kinase domain in crystalline form as claimed in claim 1, wherein said crystalline form has a space group of $P4_3$.

4. A method of ErbB4 inhibitor design, comprising:

generating a three dimensional computer model which represents ErbB4 kinase domain in liganded form, said kinase domain described by the amino acid sequence of SEQ ID NO: 1 and having the structural coordinates of Table 2;

evaluating compounds as potential ErbB4 inhibitors using said model; and

selecting compounds for further testing based on said evaluation.

5. A method of ErbB4 inhibitor design, comprising:

generating a three dimensional computer model which represents a ErbB4 kinase domain in liganded form, said kinase domain described by the

amino acid sequence of SEQ ID NO: 1 and having the structural coordinates of Table 2;

evaluating compounds as potential ErbB4 inhibitors using said model; wherein said evaluation comprises identifying compounds capable of at least one of the following ErbB4 kinase domain/compound interactions:

(iv) one or more interactions with amino acid residues of the ErbB4 kinase domain hinge region;

(v) one or more interactions with amino acid residues of the ErbB4 kinase domain adenine pocket,

(iii) one or more interactions with amino acid residues of the ErbB4 kinase sugar pocket,

(iv) one or more interactions with amino acid residues of the ErbB4 kinase domain back pocket, and

(v) one or more interactions with amino acid residues of the ErbB4 kinase domain solvent interface; and

selecting compounds for further testing based on said evaluation.

6. A method of ErbB4 inhibitor design, comprising:

generating a three dimensional computer model which represents a ErbB4 kinase domain in liganded form, said kinase domain described by the amino acid sequence of SEQ ID NO: 1 and having the structural coordinates of Table 2;

evaluating compounds as potential ErbB4 inhibitors using said model; wherein said evaluation comprises identifying compounds capable of at least one of the following ErbB4 kinase domain/compound interactions:

(i) one or more interactions with amino acid residues 796, 797, 798, 799, and 800;

(ii) one or more interactions with amino acid residues 724, 749, and 850;

(iii) one or more interactions with amino acid residues 848, 860, 803, 847, 732, and 725;

(iv) one or more interactions with amino acid residues 732, 749, 751, 796, 861, 860, 772, 781, 783, 794, 796, and 862; and

(v) one or more interactions with residues 801, 802, 803, 806, and 810; and

selecting compounds for further testing based on said evaluation.

7. A method of treating a disorder characterized by inappropriate ErbB4 activity in a mammal, comprising: administering to said mammal a therapeutically effective amount of a compound that can form a complex with a ErbB4 kinase domain thereby resulting in a ErbB4 kinase domain in liganded form, said kinase domain in liganded form being described by the amino acid sequence of SEQ ID NO: 1 and the structural coordinates of Table 2, wherein said complex is characterized by at least one of the following ErbB4 kinase domain/compound interactions:

(i) one or more interactions with amino acid residues of the ErbB4 kinase domain hinge region;

(ii) one or more interactions with amino acid residues of the ErbB4 kinase domain adenine pocket,

(iii) one or more interactions with amino acid residues of the ErbB4 kinase sugar pocket and phosphate region,

(iv) one or more interactions with amino acid residues of the ErbB4 kinase domain back pocket, and

(v) one or more interactions with amino acid residues of the ErbB4 kinase domain solvent interface.

8. A method of inhibiting ErbB4 in a mammal, comprising: administering to said mammal a therapeutically effective amount of a compound that can form a complex with a ErbB4 kinase domain thereby resulting in a ErbB4 kinase domain in liganded form, said kinase domain in liganded form being described by the amino acid sequence of SEQ ID NO: 1 and the structural coordinates of Table 2, wherein said complex is characterized by at least one of the following ErbB4 kinase domain/compound interactions:

(i) one or more interactions with amino acid residues of the ErbB4 kinase domain hinge region;

(ii) one or more interactions with amino acid residues of the ErbB4 kinase domain adenine pocket,

(iii) one or more interactions with amino acid residues of the ErbB4 kinase sugar pocket and phosphate region,

(iv) one or more interactions with amino acid residues of the ErbB4 kinase domain back pocket, and

(v) one or more interactions with amino acid residues of the ErbB4 kinase domain solvent interface.

9. An ErbB4 kinase domain/inhibitor complex, comprising: an ErbB4 kinase domain form being described by the amino acid sequence of SEQ ID NO: 1 and the structural coordinates of Table 2 and a compound that can form a complex with the ErbB4 kinase domain said complex is characterized by at least one of the following ErbB4 kinase domain/compound interactions:

(i) one or more interactions with amino acid residues of the ErbB4 kinase domain hinge region;

(ii) one or more interactions with amino acid residues of the ErbB4 kinase domain adenine pocket,

(iii) one or more interactions with amino acid residues of the ErbB4 kinase sugar pocket and phosphate region,

(iv) one or more interactions with amino acid residues of the ErbB4 kinase domain back pocket, and

(v) one or more interactions with amino acid residues of the ErbB4 kinase domain solvent interface.